ROBUST SUMMARIES

1-BUTENE: COMBINED REPEATED EXPOSURE TOXICITY, REPRODUCTION AND NEUROTOXICITY SCREENING IN RATS VIA WHOLE-BODY INHALATION EXPOSURES

Repeated Dose Toxicity

Test Article	
Remarks	1-BUTENE Purity: =99% CAS number: 106-98-9
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures.
GLP	Yes.
Year	2003
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (gas).
Duration of test	28 days
Doses/concentration levels	0, 500, 2000, or 8000 ppm
Sex	12 males, 12 females per dose group for main study group
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 males, 12 females, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Mean values of all exposure groups were compared to the mean value for the control group at each time interval. For all parameters except for organ weights, the standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional testing was performed using Dunnett's t-test to determine which means were significantly different from the control. Organ weight data was analyzed only by parametric methods. Bartlett's test was performed to determine if groups had equal variances. The standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional tests were used to determine which means were significantly different from the control: Dunnett's t-test for homogeneous data, or Cochran and Cox's modified t-test for non-homogeneous data. All t-tests were conducted at the 5% and 1% significance levels. Motor Activity Data was analyzed using split-plot repeated measures ANOVA with model terms for group, animal within group, interval and group by interval interaction. If the group x interval interaction was statistically significant (p=0.05), indicating non-parallelism in the behavioral profile between groups, a separate one-way ANOVA for group effects was performed at each interval. If the response data passed on the parallel hypothesis, an ANOVA (using summed responses over intervals) was used to test for the overall treatment effect which constituted the level hypothesis. If any significant overall treatment group effect was found by any of the above

	ANOVAs, Dunnett's t-test was used to find groups that differed from control. Analyses were performed for sexes separately and combined. Treatment group effects were deemed significant at the p=0.05 level. Plots, tables, listings, and analyses were generated using SAS® version 6.12 for WINDOWS. Analyses were conducted by CATO Research, 200 Westpark Corporate Center, 4364 South Alston Avenue, Durham, NC 27713-2280. The Testing Facility was responsible for the GLP compliance of this subcontractor.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats (approximately 8 weeks old) were exposed to the test article as a gas daily by inhalation for approximately six hours/day at exposure levels of 0, 500, 2000, or 8000 ppm. The main study (repeated-exposure general toxicity and neurotoxicity endpoints) males and females were exposed for 28 days, respectively. Effects on general toxicity, neurobehavioral activity, clinical chemistry, coagulation and hematology were evaluated. In addition, a gross necropsy with extensive histopathologic examination of tissues was conducted. The study also contained reproductive and developmental toxicity satellite groups (summarized separately).
Results	
NOAEL (NOEL)	8000 ppm .
LOAEL (LOEL)	Not applicable.
Remarks	The mean (± standard deviation) analytical (GC) concentrations for the control and the exposure groups were as follows: 0 ± 0, 524 ± 40, 2062 ± 126 and 8271 ± 683 ppm. The analytically measured exposure levels of the airborne test article were reasonably close to the targeted exposure levels. Chamber environmental conditions averaged 23°C temperature and 57% relative humidity. Mean particle size distribution measurements for the exposure indicated that the atmospheres were gas only, as expected, since there was no substantial difference between the test article chambers and the Air Control chambers. There was no effect of treatment on survival. All animals survived until the termination of the study. The test animals were unremarkable during the exposure periods (in-chamber) and during non-exposure periods. There were no exposure-related differences in body weights or weight changes or feed consumption in the test article exposed animals compared to the Air Control animals. There was no apparent exposure-related effect on motor activity or function observational battery parameters for either sex in this study. There were no exposure-related differences in hematology or coagulation values or clinical chemistry values in test article exposed animals compared to the Air Control animals at the terminal interval. There were no exposure-related differences in macroscopic postmortem evaluations or organ weights in the test article exposed animals compared to the Air Control animals. There were no microscopic findings considered to be related to exposure to 1-Butene. In comparison with controls, there was a slightly increased incidence and severity of mixed inflammatory cells in the cecal mucosa of rats exposed to 1-Butene at exposure levels of 2000 ppm and above. The cecal mucosa normally contains a small population of mixed inflammatory cells, which acts as a natural

	defense mechanism against ingested substances or organisms. Increased numbers of inflammatory cells are sometimes seen as a normal spontaneous finding, and this was evident in a few males and females from the control group in this study. Since the finding was present in the control group and there was no clear exposure level response relationship in the treated groups, the increased incidence is considered to be fortuitous and unlikely to be related to treatment with 1-Butene. Other microscopic findings occurred sporadically or showed a similar incidence in control and 1-Butene-treated animals. None were considered to be associated with exposure to the test article.
Conclusions	Exposure of male and female rats to target concentrations of 500, 2000 and 8000 ppm of 1-Butene resulted in no general systemic effects or effects on reproductive performance. Therefore, a no observed effect level (NOEL) of 8000 ppm was determined.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Hoffman G.M. (2003). 1-Butene: A combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures. Report of Huntingdon Life Sciences conducted for the American Chemistry Council Olefins Panel. Report reference: 02-4224
Other	
Last changed	21 May 2003 Robust summary prepared by contractor to Olefins Panel

Toxicity to Reproduction

Test Article	
Remarks	1-BUTENE Purity: =99% CAS number: 106-98-9
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures.
GLP	Yes.
Year	2003
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (gas).
Duration of test	Two weeks prior to breeding, during breeding, and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until lactation day 4.
Doses/concentration levels	0, 500, 2000, or 8000 ppm
Sex	12 females per dose group for this satellite study.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 females, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Mean values of all exposure groups were compared to the mean value for the control group at each time interval. For all parameters except for organ weights, the standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional testing was performed using Dunnett's t-test to determine which means were significantly different from the control. Organ weight data was analyzed only by parametric methods. Bartlett's test was performed to determine if groups had equal variances. The standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional tests were used to determine which means were significantly different from the control: Dunnett's t-test for homogeneous data, or Cochran and Cox's modified t-test for non-homogeneous data. All t-tests were conducted at the 5% and 1% significance levels. For incidence data, a Fisher Exact Test with Bonferonni correction was performed to identify differences between the control and treatment groups.
Test Conditions	Satellite groups of 12 female Sprague Dawley rats (approximately 8 weeks old) were exposed to the test article as a gas daily by inhalation for approximately six hours/day at exposure levels of 0, 500, 2000, or 8000 ppm. The study design included a main study for repeated dose toxic ity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were exposed for two weeks prior to breeding, during breeding, and continuing through day 19 of gestation. Males from the main study were used to breed these females. The dams

	were allowed to deliver their litters, which were retained until lactation day 4. Effects on general toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 4. Litter size, pup survival, sex, body weight, and the presence of gross external malformations were assessed in the offspring. In addition to the repeated dose toxicity end points assessed (discussed separately for female rats), this study would detect effects on conception, development of the conceptus and parturition and pup survival to lactation Day 4
Results	
NOAEL (NOEL)	8000 ppm.
LOAEL (LOEL)	Not applicable.
Remarks	The mean (± standard deviation) analytical (GC) concentrations for the control and the exposure groups were as follows: 0 ± 0, 524 ± 40, 2062 ± 126 and 8271 ± 683 ppm. The analytically measured exposure levels of the airborne test article were reasonably close to the targeted exposure levels. Chamber environmental conditions averaged 23°C temperature and 57% relative humidity. Mean particle size distribution measurements for the exposure indicated that the atmospheres were gas only, as expected, since there was no substantial difference between the test article chambers and the Air Control chambers. There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption was observed at any dose level tested throughout the duration of the study. All mated female animals (except one animal in the 2000 ppm group) were found pregnant and delivered live pups. Mating indices for the male rats treated with the test article were comparable to the Air Control group. Mating, fertility and gestation indices for the female rats treated with the test article were comparable to the Air Control group. Most of the females mated at the first opportunity. There were also no treatment-related differences in the other reproductive parameters up to the time of parturition including the percent of females completing delivery and the duration of gestation, when compared to the Air Control group. There were no treatment related differences in all parturition parameters including the total number of pups delivered, the number of pups dying, the viability (4 day survival) index, the number of implantation sites and corpora lutea per dam, the pup sex ratio and the number of live pups/litter, when compared to the Air Control group.
Conclusions	Repeated inhalation exposure of 1-Butene to female Sprague Dawley rats at levels of 0, 500, 2000, or 8000 ppm produced no evidence of adverse effects on any measures of reproductive function. Based on these data, the no-observable-effect level (NOEL) for reproductive toxicity was 8000 ppm, the highest concentration tested.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Hoffman G.M. (2003). 1-Butene: A combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures. Report of Huntingdon Life Sciences conducted for the American Chemistry Council Olefins Panel.

Other	
Last changed	21 May 2003 Robust summary prepared by contractor to Olefins Panel

Developmental Toxicity/Teratogenicity

Test Article	
Remarks	1-BUTENE Purity: =99% CAS number: 106-98-9
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures.
GLP	Yes.
Year	2003
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (gas).
Duration of test	Two weeks prior to breeding, during breeding, and continuing through day 19 of gestation. The dams were then allowed to deliver their litters, which were retained until lactation day 4.
Doses/concentration levels	0, 500, 2000, or 8000 ppm
Sex	12 females per group.
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 females, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Mean values of all exposure groups were compared to the mean value for the control group at each time interval. For all parameters except for organ weights, the standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional testing was performed using Dunnett's t-test to determine which means were significantly different from the control. Organ weight data was analyzed only by parametric methods. Bartlett's test was performed to determine if groups had equal variances. The standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional tests were used to determine which means were significantly different from the control: Dunnett's t-test for homogeneous data, or Cochran and Cox's modified t-test for non-homogeneous data. All t-tests were conducted at the 5% and 1% significance levels. For incidence data, a Fisher Exact Test with Bonferonni correction was performed to identify differences between the control and treatment groups.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats (approximately 8 weeks old) were exposed to the test article as a gas daily by inhalation for approximately six hours/day at exposure levels of 0, 500, 2000, or 8000 ppm. The study design included a main study for repeated dose toxicity end points (summarized separately) and reproductive / developmental toxicity satellite groups of 12 females per exposure level. The reproductive and developmental toxicity satellite groups were exposed for two weeks prior to breeding, during breeding (up to two weeks), and continuing until day 19 of gestation. Males from the main study were used to breed these females. The dams were allowed to deliver their litters, which were retained until lactation day 4. Effects on general

	toxicity, gonadal function, mating behavior, implantation, and general fertility were evaluated in the satellite group adults, followed by a gross necropsy of the satellite group females on lactation day 4. Litter size, pup survival, sex, body weight, and the presence of gross external malformations were assessed in the offspring.
Results	
NOAEL (NOEL)	8000 ppm.
LOAEL (LOEL)	Not applicable.
Remarks	The mean (± standard deviation) analytical (GC) concentrations for the control and the exposure groups were as follows: 0 ± 0, 524 ± 40, 2062 ± 126 and 8271 ± 683 ppm. The analytically measured exposure levels of the airborne test article were reasonably close to the targeted exposure levels. Chamber environmental conditions averaged 23°C temperature and 57% relative humidity. Mean particle size distribution measurements for the exposure indicated that the atmospheres were gas only, as expected, since there was no substantial difference between the test article chambers and the Air Control chambers. There were no deaths or treatment-related clinical observations noted. No significant differences in parental body weights, body weight gains or feed consumption was observed at any dose level tested throughout the duration of the study. There were no treatment-related effects at any dose level on any of the reproductive parameters evaluated in this study. These included measures of reproductive performance (mating, conception and fertility, time to mating, gestation length, litter size), offspring survival (gestation and postnatal survival indices, percent pre- and post-implantation loss), pup body weight and pup sex ratio. The pups were unremarkable during the lactation period. There were no exposure-related differences in body weights or weight gains in pups feeding from test article exposed animals compared to the pups feeding from Air Control animals. There were no exposure-related differences in macroscopic postmortem evaluations in the pups feeding from the test article exposed animals compared to the pups feeding from Air Control animals.
Conclusions	Repeated inhalation exposure of 1-Butene to male and female Sprague Dawley rats at levels of 0, 500, 2000 and 8000 ppm produced no evidence of developmental toxicity or teratogenicity, as assessed in the OECD 422 study design. Based on these data, the no-observable-effect level (NOEL) for developmental toxicity was 8000 ppm, the highest concentration tested.
Data Quality	
Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Hoffman G.M. (2003). 1-Butene: A combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures. Report of Huntingdon Life Sciences conducted for the American Chemistry Council Olefins Panel.
Other	
Last changed	21 May 2003 Robust summary prepared by contractor to Olefins Panel

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E261

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Melting Point

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential melting point range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point of substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the melting point range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated MP (°C) / Measured* MP (°C) Isobutane: -132.55 / -138.3 n-butane: -120.28 / -138.2 isobutylene: -130.88 / -140.4 cis-butene-2: -120.41 / -105.5 trans-butene-2: -120.41 / -105.5 butene-1: -121.74 / -145.0 1,2-butadiene: -117.86 / -136.2 1,3-butadiene: -123.21 / -108.9 * Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E261

Conclusion:	Based on calculated constituent data, substances in this category can have a melting range of -117.86 to -120.28 °C. Based on measured constituent data, substances in this category can have a melting range of -145.0 to -105.5°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Melting Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E223

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Biodegradation

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Inoculum:	Not applicable
Exposure Period:	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Not applicable
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Not applicable
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product

Test Substance: (cont'd)	Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process, and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, biodegradation will not contribute significantly to the loss of chemicals in substances from the Low 1,3-Butadiene C4 category (C4 refers to a chemical with 4 carbons). The Low 1,3-Butadiene C4 category includes seven process streams: • **C4 Raffinate 1** • **C4 Raffinate 2** • **Isobutylene** • **Butene-1** • **C4 Raffinate 3** • **Butane** • **Catalytic Butylenes** Eight CAS numbers (see Test Substance) identify substances derived from these process streams. The substances contain various chemicals composed of carbon and hydrogen. As discussed below, substances in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that substances from this category will partition to environmental compartments where they could be degraded by bacteria. **The Low 1,3-Butadiene C4 Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and complex

	hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are: • **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate. • **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes. • **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure. • **Butene-1** is produced by distillation from isobutylene plant raffinate.

- **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane.
- **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3.
- **Catalytic Butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit.

Biodegradation of Hydrocarbons

Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.

Substances in the Low 1,3-Butadiene C4 Category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C5. Consequently, their availability to microbial degraders will be significantly limited.

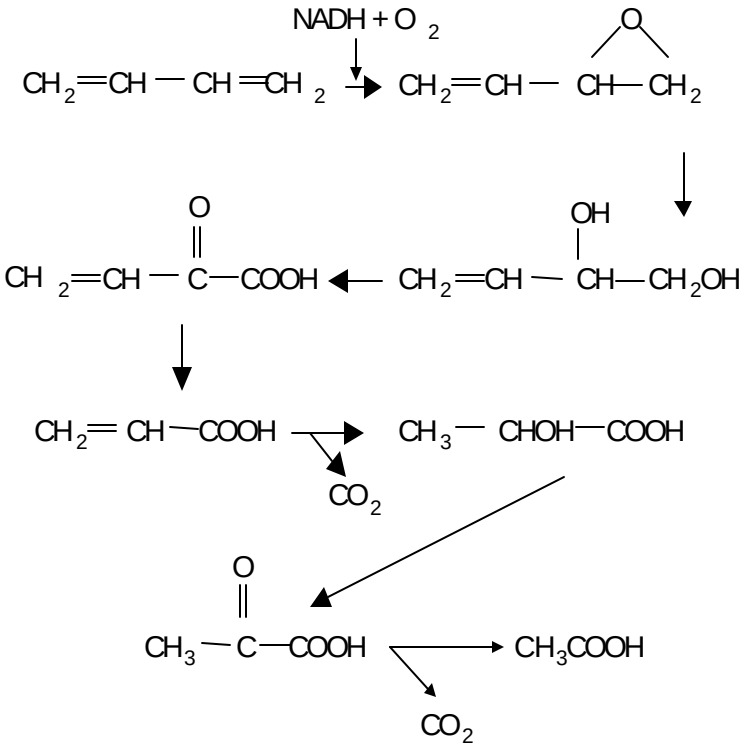
Component chemicals from all seven process streams in this category are simple hydrocarbons, the majority of which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical attack) for specific degradation rates of selected chemicals from this category; AOP data were developed for this category under the HPV Chemical Program]. All chemicals from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment.

Substances from the Low 1,3-Butadiene C4 Category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for chemicals in this category that demonstrates that they can be biodegraded.

Watkinson and Morgan (6) state that microbial metabolism of aliphatic alkenes, such as those in the Low 1,3-Butadiene C4 Category, can be initiated by attack at the double bond. Four degradative processes have been identified:

- oxygenase attack upon a terminal methyl group to the corresponding unsaturated alcohol and acid,
- subterminal oxygenase attack to the corresponding alcohol and acid,
- oxidation across the double bond to the corresponding epoxide, and
- oxidation across the double bond to the corresponding diol.

Experimental studies to determine a catabolic pathway for 1,3-butadiene as mediated by a *Nocardia* sp. (3), for example, resulted in the following proposed series of reactions:



The intermediary metabolic steps depicted above result in the production of acetic acid, CH3COOH, which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (2).

The potential biodegradability of some of the other components including butane, 1-butene, and 2-butene has been summarized and metabolic pathways leading to their biodegradation have been

	described (4, 5). These chemicals have been shown to biodegrade to high extents such that if they were to partition to either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment. In summary, because the C4 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Chemical components of this category that are greater than C4 also have a potential to partition to the air to a great extent, where they will also degrade rapidly in a similar manner. However, they also have a potential to partition to aquatic and terrestrial environments where they are subject to biological processes that can result in their rapid biodegradation. Overall, substances from this category and their component chemicals are expected to degrade rapidly in the environment and not persist. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA. 3. Watkinson, R.J. and H.J. Somerville. 1976. The Microbial Utilization of Butadiene. Shell Research Limited, Sittingbourne Research Centre, Kent, UK. 4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA. 5. Hartmans, S. 1993. Biodegradation of chlorinated and unsaturated hydrocarbons in relation to biological waste-gas treatment. Thesis Wageningen University. NL. 6. Watkinson, R.J. and P. Morgan. 1990. Physiology of aliphatic hydrocarbon-degrading microorganisms. *Biodegradation*. 1:79-92.
Reliability:	Not applicable
Reference:	American Chemistry Council, Olefins Panel. 2002. Biodegradation: Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is an option in the "test substance" pick list within the IUCLID data entry field for "biodegradation". Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E260

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Boiling Point

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential boiling point range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the boiling point range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E260

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated BP (°C) / Measured* BP (°C) Isobutane 3.21 -11.7 n-butane 19.58 -0.5 isobutylene 10.18 -6.9 cis-butene-2 27.82 0.8 trans-butene-2 27.82 0.8 butene-1 17.57 -1.3 1,2-butadiene 19.71 10.9 1,3-butadiene 15.55 -4.4 * Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E260

Conclusion:	Based on calculated constituent data, substances in this category can have a boiling range of 3.21 to 27.82°C @ 760 mm Hg. Based on measured constituent data, substances in this category can have a boiling range of -11.7 to 10.9°C @ 760 mm Hg.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 8 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Boiling Point. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E248

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Alga Toxicity

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Green Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Alga (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:*	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent / Calculated log K_{ow} / Measured* log K_{ow} Isobutane: 2.23 / 2.76 n-butane: 2.31 / 2.89 isobutylene: 2.23 / 2.34 cis-butene-2: 2.09 / 2.31 trans-butene-2: 2.09 / 2.33 butene-1: 2.17 / 2.40 1,2-butadiene: 2.06 / na 1,3-butadiene: 2.03 / 1.99 na = not available

Test Conditions: (cont'd) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated alga acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent / Calculated log K_{ow} / Alga Toxicity 96-hr EC50 (mg/L) Isobutane: 2.23; 18.06 n-butane: 2.31; 15.35 isobutylene: 2.23; 17.44 cis-butene-2: 2.09; 23.19 trans-butene-2: 2.09; 23.19 butene-1: 2.17; 19.71 1,2-butadiene: 2.06; 23.77 1,3-butadiene: 2.03; 25.27

Results: (cont'd) **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Substance Constituent / Measured* log K_{ow} / Alga Toxicity 96-hr EC50 (mg/L) Isobutane: 2.76; 6.13 n-butane: 2.89; 4.71 isobutylene: 2.34; 13.94 cis-butene-2: 2.31; 14.81 trans-butene-2: 2.33; 14.22 butene-1: 2.40; 12.33 1,2-butadiene: na; na 1,3-butadiene: 1.99; 27.42 na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. The data represent a potential acute toxicity range for substances represented by the 8 CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

	1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 15.35 to 25.27 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 4.71 to 27.42 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic plants based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Acute Toxicity to Aquatic Plants. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E250

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Fish Acute Toxicity

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Fish (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:*	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent / Calculated log K_{ow} / Measured* log K_{ow} Isobutane: 2.23 / 2.76 n-butane: 2.31 / 2.89 isobutylene: 2.23 / 2.34 cis-butene-2: 2.09 / 2.31 trans-butene-2: 2.09 / 2.33 butene-1: 2.17 / 2.40 1,2-butadiene: 2.06 / na 1,3-butadiene: 2.03 / 1.99 na = not available

Test Conditions: (cont'd) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated fish acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent — Calculated log K_{ow} — Fish Acute 96-hr LC50 (mg/L) Isobutane — 2.23 — 26.19 n-butane — 2.31 — 22.03 isobutylene — 2.23 — 25.28 cis-butene-2 — 2.09 — 34.23 trans-butene-2 — 2.09 — 34.23 butene-1 — 2.17 — 28.79 1,2-butadiene — 2.06 — 35.22 1,3-butadiene — 2.03 — 37.59

Results: (cont'd)

Units/Value:

Note: Deviations from protocol or guideline, analytical method, biological observations, control survival

Substance Constituent	Measured* log K_{ow}	Fish Acute 96-hr LC50 (mg/L)
Isobutane	2.76	8.32
n-butane	2.89	6.28
isobutylene	2.34	19.93
cis-butene-2	2.31	21.26
trans-butene-2	2.33	20.36
butene-1	2.40	17.50
1,2-butadiene	na	na
1,3-butadiene	1.99	40.98

na = not available

* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.

The data represent a potential acute toxicity range for substances represented by the eight CAS numbers under Test Substance.

Test Substance:

The Low 1,3-Butadiene C4 Category includes the following CAS numbers:

106-97-8	Butane
106-98-9	1-Butene
115-11-7	1-Propene,2-methyl
25167-67-3	Butenes
68477-42-9	Gases, petroleum, extractive, C3-5, butene-isobutylene-rich
68477-83-8	Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed
68527-19-5	Hydrocarbons, C1-4, debutanizer fraction
68606-31-5	Hydrocarbons C3-5, butadiene purification by-product

Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins.

More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E250

	1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 22.03 to 37.59 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 6.28 to 40.98 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to fish based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Acute Toxicity to Fish. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E249

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Daphnid Acute Toxicity

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline*:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Daphnid (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:*	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent / Calculated log K_{ow} / Measured* log K_{ow} Isobutane: 2.23 / 2.76 n-butane: 2.31 / 2.89 isobutylene: 2.23 / 2.34 cis-butene-2: 2.09 / 2.31 trans-butene-2: 2.09 / 2.33 butene-1: 2.17 / 2.40 1,2-butadiene: 2.06 / na 1,3-butadiene: 2.03 / 1.99 na = not available

Test Conditions: (cont'd) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated daphnid acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent / Calculated log K_{ow} / Daphnid Acute 48-hr LC50 (mg/L) Isobutane: 2.23; 28.51 n-butane: 2.31; 24.11 isobutylene: 2.23; 27.53 cis-butene-2: 2.09; 36.91 trans-butene-2: 2.09; 36.91 butene-1: 2.17; 31.21 1,2-butadiene: 2.06; 37.89 1,3-butadiene: 2.03; 40.27

Results: (cont'd)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**

Substance Constituent	Measured* log K_{ow}	Daphnid Acute 48-hr LC50 (mg/L)
Isobutane	2.76	9.39
n-butane	2.89	7.15
isobutylene	2.34	21.86
cis-butene-2	2.31	23.28
trans-butene-2	2.33	22.32
butene-1	2.40	19.28
1,2-butadiene	na	na
1,3-butadiene	1.99	43.88

na = not available

* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.

The data represent a potential acute toxicity range for substances represented by the eight CAS numbers under Test Substance.

Test Substance:

The Low 1,3-Butadiene C4 Category includes the following CAS numbers:

106-97-8	Butane
106-98-9	1-Butene
115-11-7	1-Propene,2-methyl
25167-67-3	Butenes
68477-42-9	Gases, petroleum, extractive, C3-5, butene-isobutylene-rich
68477-83-8	Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed
68527-19-5	Hydrocarbons, C1-4, debutanizer fraction
68606-31-5	Hydrocarbons C3-5, butadiene purification by-product

Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins.

More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E249

	1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 24.11 to 40.27 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 7.15 to 43.88 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic invertebrates based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Acute Toxicity to Aquatic Invertebrates. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.:OP E268

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Photodegradation (Direct)

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable
Direct Photolysis:** • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Low 1,3-Butadiene C4 Category (C4 refers to a chemical with 4 carbons). The Low 1,3-Butadiene C4 Category includes seven process streams: • **C4 Raffinate 1** • **C4 Raffinate 2** • **Isobutylene** • **Butene-1** • **C4 Raffinate 3** • **Butane** • **Catalytic butylenes**

Eight CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis.

The Low 1,3-Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The typical compositions of the streams in this category are shown in Table 2.

The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are:

- **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate.
- **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes.

	• **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure. • **Butene-1** is produced by distillation from isobutylene plant raffinate. • **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane. • **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3. • **Catalytic butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit. **<u>Photolysis of Hydrocarbons</u>** The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state. The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule. The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

	A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max}) and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2): **l below 290 nm** / **l above 290 nm** Hydrocarbon — l_{max} — e — l_{max} — e Ethylene — 193 — 10,000 — - — - 1,3-Butadiene — 217 — 2,090 — - — - Benzene — 255 — 215 — - — - Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Low 1,3-Butadiene C4 Category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2). Substances in the Low 1,3-Butadiene C4 Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.:OP E268

Degradation Products:** • **Note: Identification, concentration**	Unknown
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the Low 1,3-Butadiene C4 Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2002. Photodegradation (Direct): Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Direct). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E267

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Hydrolysis (Stability in Water)

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category products arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and

	other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these products contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the Low 1,3-Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes seven process streams: • **C4 Raffinate 1** • **C4 Raffinate 2** • **Isobutylene** • **Butene-1** • **C4 Raffinate 3** • **Butane** • **Catalytic butylenes** Eight CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. **The Low 1,3-Butadiene C4 Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4.

	The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are: • **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate. • **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes. • **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure. • **Butene-1** is produced by distillation from isobutylene plant raffinate. • **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane. • **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3.

- **Catalytic butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment.

Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Low 1,3-Butadiene C4 Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4).

The substances in the Low 1,3-Butadiene C4 Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Low 1,3-Butadiene C4 Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment.

References

1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

	2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	Not applicable
Reference:	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Hydrolysis. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E270

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Photodegradation (Indirect)

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis:** **Results: half-life, % degradation, quantum yield**	Not applicable

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E270

Indirect Photolysis:** • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The Low 1,3-Butadiene C4 Category** Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. Commercial products in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-8 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The eight chemicals selected to represent the atmospheric oxidation potential of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH-radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals. Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E270

Indirect Photolysis: (cont'd)** **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Chemical / Calculated* half-life (hrs) / OH- Rate Constant (cm^3/molecule-sec) Isobutane 52.6 $2.4\ E^{-12}$ n-butane 48.8 $2.6\ E^{-12}$ isobutylene 2.5 $51.7\ E^{-12}$ cis-butene-2 2.3 $56.7\ E^{-12}$ trans-butene-2 2.0 $64.3\ E^{-12}$ butene-1 4.7 $27.4\ E^{-12}$ 1,2-butadiene 4.1 $31.1\ E^{-12}$ 1,3-butadiene 1.9 $66.6\ E^{-12}$ * Atmospheric half-life values are based on a 12-hr day. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001). References: 1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442. 2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY. 3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299. 4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Degradation Products:** • **Note: Identification, concentration**	Unknown

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5

Robust Summary No.: OP E270

Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 1.9 to 52.6 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 8 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Photodegradation (Indirect). Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

** In IUCLID, provide additional discussion if needed in the results freetext

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E263

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Partition Coefficient

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential log K_{ow} range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the log K_{ow} range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated log K_{ow} @ 25°C / Measured* log K_{ow} @ 25°C Isobutane: 2.23 / 2.76 n-butane: 2.31 / 2.89 isobutylene: 2.23 / 2.34 cis-butene-2: 2.09 / 2.31 trans-butene-2: 2.09 / 2.33 butene-1: 2.17 / 2.40 1,2-butadiene: 2.06 / na 1,3-butadiene: 2.03 / 1.99 * Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E263

Conclusion:	Based on calculated constituent data, substances in this category can have a log K_{ow} range of 2.03 to 2.31 @ 25°C. Based on measured constituent data, substances in this category can have a log K_{ow} range of 1.99 to 2.89 @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Partition Coefficient. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E269

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Transport / Distribution (Fugacity)

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated partitioning data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential distribution for substances represented by the eight CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the environmental distribution range of this category are C4 hydrocarbons that are common across the 8 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E269

Results: (cont'd)

Units/Value:

- **Note: Deviations from protocol or guideline, analytical method.**

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution		Measured** Percent Distribution	
Chemical	Air	Water	Air	Water
Isobutane	99.99	0.01	99.99	0.01
n-butane	99.98	0.02	99.99	0.01
isobutylene	99.98	0.02	99.99	0.01
cis-butene-2	99.97	0.03	99.98	0.02
trans-butene-2	99.97	0.03	99.98	0.02
butene-1	99.98	0.02	99.99	0.01
1,2-butadiene	99.96	0.04	99.96	0.04
1,3-butadiene	99.97	0.03	99.97	0.03

* Distribution values determined using calculated input data from EPIWIN program
** Distribution values determined using input data from the EPIWIN program experimental database

Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as less than 0.01%. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals.

Test Substance:

The Low 1,3-Butadiene C4 Category includes the following CAS numbers:

106-97-8	Butane
106-98-9	1-Butene
115-11-7	1-Propene,2-methyl
25167-67-3	Butenes
68477-42-9	Gases, petroleum, extractive, C3-5, butene-isobutylene-rich
68477-83-8	Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed
68527-19-5	Hydrocarbons, C1-4, debutanizer fraction
68606-31-5	Hydrocarbons C3-5, butadiene purification by-product

Test Substance: (cont'd)	Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the eight CAS numbers listed under Test Substance. Substances in the Low 1,3-Butadiene C4 Category are calculated to partition primarily to air with a smaller percentage partitioning to water. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E269

Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Transport-Distribution. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E262

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Vapor Pressure

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential vapor pressure for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure of substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the vapor pressure range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E262

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated VP (hPa @ 25°C) / Measured* VP (hPa @ 25°C) Isobutane: 3.45 E^3 / 3.08 E^3 n-butane: 2.41 E^3 / 2.43 E^3 isobutylene: 2.97 E^3 / 3.08 E^3 cis-butene-2: 2.31 E^3 / 2.33 E^3 trans-butene-2: 2.31 E^3 / 2.33 E^3 butene-1: 2.48 E^3 / 3.00 E^3 1,2-butadiene: 1.65 E^3 / 1.68 E^3 1,3-butadiene: 2.73 E^3 / 2.81 E^3 * Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E262

Conclusion:	Based on calculated constituent data, substances in this category can have a vapor pressure range of 1.65 E^3 to 3.45 E^3 hPa @ 25°C. Based on measured constituent data, substances in this category can have a vapor pressure range of 1.68 E^3 to 3.08 E^3 hPa @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Vapor Pressure. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E264

LOW 1,3-BUTADIENE C4 ROBUST SUMMARY

Water Solubility

Test Substance*:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential water solubility range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges of substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial products in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the water solubility range of this category are C4 hydrocarbons that that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

Results: (continued) **Units/Value:** **Note: Deviations from protocol or guideline, analytical method.**	Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) Isobutane: 496.4 / 175.1 n-butane: 424.1 / 135.6 isobutylene: 495.6 / 399.2 cis-butene-2: 652.7 / 423.5 trans-butene-2: 652.7 / 407.1 butene-1: 557.7 / 354.8 1,2-butadiene: 687.8 / na 1,3-butadiene: 732.4 / 792.3 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1).

CAS No.: 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5
Robust Summary No.: OP E264

	1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a water solubility range of 424.1 to 732.4 mg/L @ 25°C. Based on measured constituent data, substances in this category can have a water solubility range of 135.6 to 792.3 mg/L @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

* Other TS is a selection option under the Test Substance pick list that is in the IUCLID entry field for Water Solublilty. Selecting this option refers the reader to information in the test substance "freetext" field to which the CAS numbers can be added.